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ScienceDirect
Linear Algebra and its Applications 429 (2008) 1679–1683
LINEAR ALGEBRA AND ITS APPLICATIONS
www.elsevier.com/locate/laa

On monotonicity of the Lanczos approximation to the matrix exponential

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Received 30 March 2008; accepted 30 April 2008
Available online 17 June 2008
Submitted by A. Frommer

Abstract

We prove strictly monotonic error decrease in the Euclidian norm of the Krylov subspace approximation of $\exp(A)\varphi$, where φ and A are respectively a vector and a symmetric matrix. In addition, we show that the norm of the approximate solution grows strictly monotonically with the subspace dimension.

AMS classification: 65F99; 15A06

Keywords: Matrix exponential; Symmetric matrix; Krylov subspace; Strictly monotonic convergence; Total positivity

1. Introduction

We want to compute

$$u(t) = e^{tA}\varphi \tag{1}$$

with $\varphi \in R^n(\|\varphi = 1\|)$, $A \in R^{n\times n}$, $A = A^*$ and scalar $t > 0$. Obviously, $u(t)$ is the solution of the initial ODE problem

$$Au - \frac{\mathrm{d}}{\mathrm{d}t}u = 0, \quad u(0) = \varphi. \tag{2}$$

We consider approximate computation of (1) using so called Spectral Lanczos Decomposition Method (SLDM), that became known since the 1980s [7,11,2, etc.], see [4] for a more up to date reference list. It can be described as follows (assuming exact arithmetic).

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doi:10.1016/j.laa.2008.04.046

Let M be the degree of the minimal polynomial of φ, i.e., the nonzero monic polynomial p of lowest degree such that $p(A)\varphi = 0$ [12]. We perform $m (m \leqslant M)$ steps of the Lanczos recursion with matrix A and initial vector φ. The Lanczos recursion produces an orthonormal basis q_i, $i = 1, \ldots, m$ on Krylov subspace $K_m = \text{span}\{\varphi, \ldots, A^{m-1}\varphi\}$. Let $\alpha_i, \beta_i (i = 1, \ldots, m)$ be the recursion coefficients as defined in [9]. Then $\beta_i > 0$ for $i = 1, \ldots, m-1$ and $\beta_M = 0$. To simplify the further notations we set $\beta_0 = 0$.

The SLDM approximate solution $u_m \in K_m$ can be written as

$$u_m = Q_m s_m(t), \quad s_m(t) = e^{tT_m} e_1,$$

where e_1 is the first unit vector, T_m is the Jacobi matrix with $\alpha_i, i = 1, \ldots, m$ and $\beta_i, i = 1, \ldots, m-1$ as the diagonal and sub-diagonal elements respectively, matrix $Q_m \in R^{n\times m}$ consists of vectors $q_i, i = 1, \ldots, m$ as the columns.

It is well known that the Conjugate Gradient (CG) method for the linear algebraic systems is the Galerkin method on the Krylov subspace. Likewise, u_m can be considered as the Galerkin approximation of the ODE system (2) on the Krylov subspace. Similar to the CG the SLDM becomes exact, if $m = M$.

A priori SLDM convergence estimates (in exact arithmetic) were obtained in [3], similar results also can be found in [5,6]. These estimates show that the SLDM converges at least with the same speed as the Tshebyshev series method proposed in [3,10], however they do not show any advantages over the latter due to the spectral adaptivity of the Galerkin method. An attempt to show the adaptivity was made in [1], where it was proven that the SLDM error is of the same order as the error of $Q_{m-2}Q^*_{m-2}u$ (the optimal approximant in Euclidean norm on K_{m-2}). However because of an unnecessary large constant this approach did not have practical implications.

One would expect monotonic convergence of u_m in some norm similar to the well known results on monotonic convergence of the CG. Here we suggest a simple convergence analysis based on the total positivity of the exponentials of the Jacobi matrices and prove strictly monotonic convergence of u_m in the Euclidean norm. In addition we show that $\|u_m\|$ grows strictly monotonically with m.

2. Main result

By construction s_m satisfies for $t \geqslant 0$ the ODE system

$$T_m s_m - \frac{\mathrm{d}}{\mathrm{d}t} s_m = 0, \quad s|_{t=0} = e_1. \tag{3}$$

The tri-diagonal matrix T_m can be viewed as a finite-difference approximation of a 1D elliptic operator, i.e., (3) can be treated as a semi-discretization of a heat equation. Let us consider an auxiliary "initial-boundary value" problem for $t \geqslant 0$ with respect to m scalar functions $r_i(t)$:

$$\beta_{i-1} r_{i-1} + \alpha_i r_i + \beta_i r_{i+1} - \frac{\mathrm{d}}{\mathrm{d}t} r_i = 0, \quad i = 1, \ldots, m \tag{4}$$

subject to the initial condition

$$r_i|_{t=0} = g_i, \quad i = 1, \ldots, m \tag{5}$$

and for $m < M$ the boundary condition

$$r_{m+1}(t) = b(t). \tag{6}$$

Since $\beta_0 = \beta_M = 0$, for uniformity of notations we can define fictitious boundary conditions $r_0 = r_{M+1} = 0$.

Lemma 1. *Problems (4)–(6) has a unique solution, more over it satisfies the total positivity condition, that can be formulated as follows. Let $g_i \geqslant 0$ for $i = 1, \ldots, m$, $b \geqslant 0$ and at least one of $g_i > 0$ or $b(t) > 0$ for $t > 0$. Then $r_i > 0$ for $t > 0$ and $i = 1, \ldots, m$.*

The above total positivity condition straightforwardly follows from the well known result on the total positivity of e^{tT_m} [8], however we give the proof of the Lemma 1 for completeness.

Proof. Systems (4)–(6) can be solved using the (first order) explicit time stepping with uniform step $\tau > 0$. The time stepping algorithm gives the following recursion:

$$\tilde{r}_i(t+\tau) = \gamma_{i-1}\tilde{r}_{i-1}(t) + \rho_i\tilde{r}_i(t) + \gamma_i\tilde{r}_{i+1}(t), \quad i = 1, \ldots, m$$

subject to the initial and boundary conditions (5) and (6), respectively, where $\gamma_i = \tau\beta_i$, $\rho_i = 1 + \tau\alpha_i$. The approximate solution $\tilde{r}_i$ will converge to the true solution as $\tau \to 0$. Because of nonnegativity of β_i we obtain $\gamma_i \geqslant 0$, also for τ small enough we have $\rho_i > 0$. So we obtain the time-stepping transition operator with the nonnegative coefficients, that gives the non-negativity of the solution.

Now, we need to prove that it is positive. We do this from the contrary, i.e., assuming that there exists $t_0 > 0$ and $i_0 \leqslant m$ such that $r_{i_0}|_{t_0} = 0$. Then $\frac{\mathrm{d}}{\mathrm{d}t}r_{i_0}(t_0) = 0$, otherwise we would have $r_{i_0}(t) < 0$ somewhere in the immediate neighborhood of t_0. Then from (4) we obtain $r_{i_0 \pm 1}(t_0) = 0$, otherwise

$$\beta_{i-1}r_{i_0-1}(t_0) + \alpha_i r_{i_0}(t_0) + \beta_i r_{i_0+1}(t_0) - \frac{\mathrm{d}}{\mathrm{d}t}r_{i_0}(t_0) > 0.$$

That implies $r_i(t_0) = 0$ for $i = 1, \ldots, m+1$, i.e., also $b(t) \equiv 0$. Then from the uniqueness of the initial problem for (4) (with the homogeneous boundary conditions) in reverse time on $[0, t_0]$ we obtain $r_i(0) = g_i = 0$ for $i = 1, \ldots, m$. $\square$

Let us denote $s_{m,i}$, $i = 1, \ldots, m$ the components of s_m.

Lemma 2. *$0 < s_{m,i}$ for any m and $s_{m,i} < s_{m+1,i}$ for $m < M$.*

Proof. First we note, that $s_{m,i}$ are the solutions of (4)–(6) with $b = 0$ and g_i being the components of e_1 for $m < M$, similarly $s_{M,i}$ are the solutions of (4) and (5), i.e., satisfy the condition of Lemma 1, so we proved the first inequality of the lemma.

To prove the second inequality we note, that for $m < M$ components of s_{m+1} give the solution of (4,5,6) with $b = s_{m+1,m+1} > 0$ and g_i being the components of e_1, so $s_{m+1,i} - s_{m,i}$ for $i \leqslant m$ satisfy (4,5,6) with $b = s_{m+1,m+1} > 0$ and all $g_i = 0$. Thus we can apply the Lemma 1 to $s_{m+1,i} - s_{m,i}$, that gives their positivity. $\square$

Theorem 1. *For any $m < M$ we have $\|u - u_{m+1}\| < \|u - u_m\|$ and $\|u_{m+1}\| > \|u_m\|$.*

Proof. From $u_m = \sum_{i=1}^{m} q_i s_{i,m}$ and exactness of u_M we obtain

$$u - u_m = u_M - u_m = \sum_{i=1}^{m} q_i(s_{M,i} - s_{m,i}) + \sum_{i=m+1}^{M} q_i s_{M,i},$$

so due to orthonormality of q_i we obtain

$$\|u - u_m\|^2 = \sum_{i=1}^{m}(s_{M,i} - s_{m,i})^2 + \sum_{i=m+1}^{M} s_{M,i}^2.$$

Assuming $m < M$, for $m + 1$ we similarly obtain

$$\|u - u_{m+1}\|^2 = \sum_{i=1}^{m+1}(s_{M,i} - s_{m+1,i})^2 + \sum_{i=m+2}^{M} s_{M,i}^2,$$

i.e.,

$$\|u - u_m\|^2 - \|u - u_{m+1}\|^2 = \sum_{i=1}^{m}[(s_{M,i} - s_{m,i})^2 - (s_{M,i} - s_{m+1,i})^2] + w,$$

where $w = s_{M,m+1}^2 - (s_{M,m+1} - s_{m+1,m+1})^2$. Due to the Lemma 2 $s_{i,M} > s_{i,m+1} > s_{i,m} > 0$, so all the terms in the square brackets are positive. Similarly $s_{m+1,M} > 0$ and $s_{m+1,M} \geq s_{m+1,m+1}$, so $w > 0$ and we proved the first inequality. The second inequality follows from $\|u_m\|^2 = \sum_{i=1}^{m} s_{i,m}^2$ and monotonicity result $0 < s_{i,m} < s_{i,m+1}$ for $i < m + 1$ of the Lemma 2. □

Remark 1. Let us denote $\lambda_{\min}$ and $\lambda_{\max}$ respectively the minimal and maximal eigenvalues of A. The obtained results can be extended to $f(A)\varphi$, that can be presented as $f(x) = \int_0^\infty w(t)e^{xt}\,dt$ with real nonnegative (nontrivial) w, assuming that $f(x)$ exists and uniformly bounded on $[\lambda_{\min}, \lambda_{\max}]$.

Remark 2. The Theorem 1 (unlike results of [1]) is not valid for the simple Lanczos algorithm (without reorthogonalization) in computer arithmetic, because q_i lose orthogonality. However all the lemmas would remain valid in this case.

Acknowledgements

The author indebted to David Ingerman, Leonid Knizhnerman, Valeria Simoncini and Mikhail Zaslavsky for very useful discussions.

References

[1] V. Druskin, A. Greenbaum, L. Knizhnerman, Using nonorthogonal Lanczos vectors in the computation of matrix functions, SIAM J. Sci. Comput. 19 (1998) 38–54.
[2] V. Druskin, L. Knizhnerman, A spectral semi-discrete method for the numerical solution of three-dimensional non-stationary electrical prospecting problems, Izv. AN USSR, ser. "Physics of Solid Earth" (8) (1988) 63–74 (in Russian; translated into English).
[3] V. Druskin, L. Knizhnerman, Two polynomial methods of calculating functions of symmetric matrices, USSR Comput. Math. Math. Phys. 29 (1989) 112–121.
[4] A. Frommer, V. Simoncini, Matrix functions, in: W. Schilders, H. van der Vorst (Eds.), Model Order Reduction: Theory, Research Aspects and Applications, Mathematics in Industry, Springer, Heidelberg, 2008.
[5] E. Gallopulos, Y. Saad, Efficient solution of parabolic equations by Krylov approximation method, SIAM J. Sci. Stat. Comput. 13 (1992) 1236–1264.
[6] M. Hochbruck, C. Lubich, On Krylov subspace approximations to the matrix exponential operator, SIAM J. Numer. Anal. 34 (1997) 1911–1925.
[7] B. Nour-Omid, Lanczos method for heat conduction analysis, Internat. J. Numer. Meth. Eng. 24 (1) (1987) 251–262.

[8] S. Karlin, Total Positivity, Stanford University Press, 1968.
[9] B. Parlett, The Symmetric Eigenvalue Problem, SIAM, 1998.
[10] H. Tal-Ezer, Spectral methods in time for parabolic problems, SIAM J. Numer. Anal. 26 (1) (1989) 1–11.
[11] H. van der Vorst, An iterative solution method for solving $f(A)x = b$ using Krylov subspace information obtained for the symmetric positive definite matrix, J. Comput. Appl. Math. 18 (2) (1987) 249–263.
[12] Y. Saad, Numerical Methods for Large Eigenvalue Problems, Manchester University Press, 1992.